

Local Limit Phenomena, Flow Compression, and Fuel Cracking Effects

Tianfeng Lu
UNIVERSITY OF CONNECTICUT

06/01/2015 Final Report

DISTRIBUTION A: Distribution approved for public release.

Air Force Research Laboratory

AF Office Of Scientific Research (AFOSR)/ RTE

Arlington, Virginia 22203

Air Force Materiel Command

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)	
28/02/2015	Final Technical Report	01/03/2013 - 28/02/2015	
4. TITLE AND SUBTITLE		5a. CONTRACT NUMBER	
Local Limit Phenomena, Flow Cor	mpression, and Fuel Cracking Effects in		
High-Speed Turbulent Flames		5b. GRANT NUMBER	
8		FA9550-13-1-0057	
		5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)		5d. PROJECT NUMBER	
Tianfeng Lu, Zhuyin Ren, Ja	cqueline H. Chen		
., , , , , , , , , , , , , , , , , , ,	·	5e. TASK NUMBER	
		5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION N	` ,	8. PERFORMING ORGANIZATION REPORT NUMBER	
Department of Mechanical Engine	O .		
University of Connecticut, Storrs,	CT 06269-3139		
Combustion Research Facility,			
Sandia National Laboratories, Live	ermore, CA 94550		
9. SPONSORING / MONITORING AG	ENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)	
AFOSR/JA (703) 696-9500			
875 NORTH RANDOLPH S	STREET		
SUITE 325, ROOM 3112		11. SPONSOR/MONITOR'S REPORT	
		NUMBER(S)	

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The objective of the proposed research is to understand the roles of local limit phenomena, e.g. local extinction and reignition, interactions between flow compression and fast-reaction induced dilatation (reaction compression), and to identify the rate-limiting fuel oxidation pathways in high-speed turbulent flames. To achieve this objective, systematic computational diagnostics were developed and performed based on elementary flames and turbulent flames simulated with direct numerical simulations (DNS). During the current reporting period, progress has been made in the following tasks: 1) Computational diagnostics were developed to identify local ignition and extinction and reaction fronts in turbulent flames simulated using DNS. 2) Effects of surrogate jet fuel composition and fuel cracking reactions on high temperature combustion were studied using a bifurcation analysis. 3) Reduced mechanisms for high-temperature combustion of n-butane and n-dodecane with lumped fuel cracking reactions were developed and validated. 4) 2-D DNS was performed to investigate the fuel cracking effects in high temperature and strongly turbulent premixed flames. 5) A highly efficient ODE solver, dynamic adaptive hybrid integration, was developed for stiff chemistry.

15. SUBJECT TERMS

chemical explosive mode analysis (CEMA); computational diagnostics; direct numerical simulation; fuel cracking; reduced mechanism; jet fuel surrogate

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified	UL	23	19b. TELEPHONE NUMBER (include area code)

LOCAL LIMIT PHENOMENA, FLOW COMPRESSION, AND FUEL CRACKING EFFECTS IN HIGH-SPEED TURBULENT FLAMES

(AFOSR Grant No. FA9550-13-1-0057)

Tianfeng Lu, Zhuyin Ren
Department of Mechanical Engineering
University of Connecticut, Storrs, CT 06269-3139

Jacqueline H. Chen
Combustion Research Facility
Sandia National Laboratories, Livermore, CA 94550

SUMMARY/OVERVIEW

The objective of the proposed research is to understand the roles of local limit phenomena, e.g. local extinction and re-ignition, interactions between flow compression and fast-reaction induced dilatation (reaction compression), and to identify the rate-limiting fuel oxidation pathways in high-speed turbulent flames. To achieve this objective, systematic computational diagnostics were developed and performed based on elementary flames and turbulent flames simulated with direct numerical simulations (DNS). During the current reporting period, progress has been made in the following tasks: 1) Computational diagnostics were developed to identify local ignition and extinction and reaction fronts in turbulent flames simulated using DNS. 2) Effects of surrogate jet fuel composition and fuel cracking reactions on high temperature combustion were studied using a bifurcation analysis. 3) Reduced mechanisms for high-temperature combustion of n-butane and n-dodecane with lumped fuel cracking reactions were developed and validated. 4) 2-D DNS was performed to investigate the fuel cracking effects in high temperature and strongly turbulent premixed flames. 5) A highly efficient ODE solver, dynamic adaptive hybrid integration (AHI), was developed for stiff chemistry.

TECHNICAL DISCUSSION

1. Chemical explosive mode analysis (CEMA) for computational flame diagnostics

The method of chemical explosive mode analysis (CEMA) is a systematic approach to identify limit flame phenomena, including local ignition, extinction, and premixed and non-premixed reaction fronts, in both laminar and turbulent flames. A chemical explosive mode (CEM) is an eigenmode of the chemical Jacobian associated with a positive eigenvalue. CEM is a chemical property that distinguishes a combustible mixture from other substances, and the interaction between CEM and the mixing processes can result in local ignition and extinction. Therefore CEMA is an effective diagnostics to identify local limit phenomena.

In the present project, CEMA is used to identify and track the local ignition and extinction in turbulent flames simulated by DNS at Sandia. Two DNS datasets previously generated at Sandia are employed for the analysis: a non-premixed temporal jet flame of ethylene-air diluted with N₂ (DNS by D.O. Lignell), and a premixed turbulent counterflow flame of hydrogen-air supported by super-adiabatic hot products (DNS by S. Lyra). The two DNS datasets show significantly different flame extinction behaviors: the non-premixed ethylene jet flame is characterized by a folded S-curve, which is typical in practical combustors, and the counterflow flame features a stretched S-curve with the flame being support by adiabatic hot-product (50K above adiabatic flame temperature). Both the DNS datasets were generated from Sandia's multi-million-CPU-hour supercomputing and are high fidelity data sources for computational diagnostic benchmarking and turbulent combustion model creation and validation.

The CEMA result for the non-premixed temporal jet flame for ethylene/air is shown in Fig. 1 for the center-cut plane of the 3-D DNS at t=0.1ms. Extensive local extinction can be observed on the temperature plot as indicated by the discontinuities on the non-premixed reaction fronts (high-T layer indicated by the dark red colors). On the CEMA plots, the near- and post-

extinction mixtures are unambiguously captured as the red spots (with CEM) on the eigenvalue plot and the yellow-red spots on the Da plot, as mixtures becomes explosive at near-extinction conditions where the incomplete combustion results in high concentrations of reactants while the temperature is still high. Compared with the temperature based criteria, the CEMA based approach is more robust and universal to capture the local extinction (and possible re-ignition).

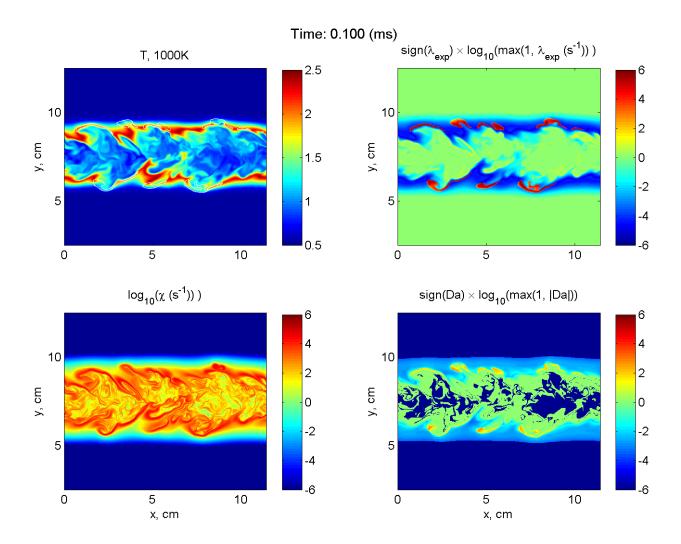


Figure 1: A 2-D snapshot of a 3-D DNS of a non-premixed temporal jet of N₂-dilited ethylene-air experiencing substantial local extinction. The local extinction was captured by CEMA on the eigenvalue plot (as red spots) and the Da plot (yellow-red spots).

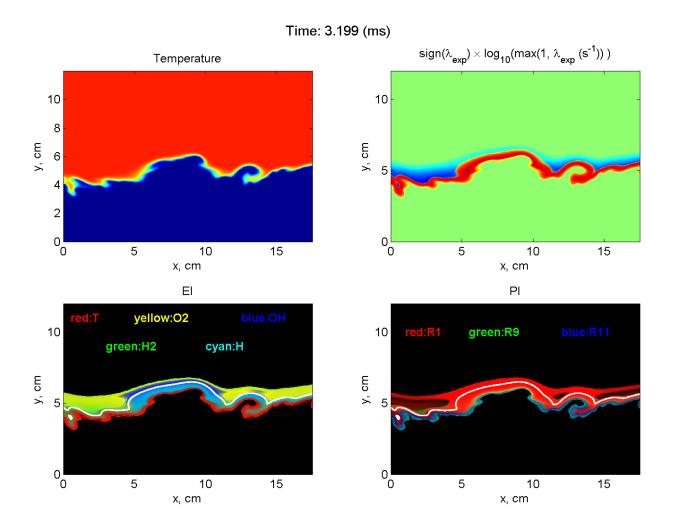


Figure 2: A 2-D snapshot from a 3-D DNS of a premixed counterflow flame for hydrogen/air supported by super-adiabatic hot product (red zones on the temperature plot). A flame hole is visualized by CEMA on the eigenvalue plot (with the dark-blue post-reaction zone missing) and the species explosion index (EI) plot. The controlling reactions are further identified by the reaction's participation index (PI).

The CEMA results on the counterflow flame of premixed hydrogen/air are shown in Fig. 2. It is noted that the hydrogen flame is supported by super-adiabatic hot products (50K above the adiabatic flame temperature), such that local flame extinction is not discernable from the temperature plot. In contrast, CEMA successfully identified the flame hole (local extinction)

through the identification of the missing post-flame-zone in the flame hole as shown on the eigenvalue plot of Fig. 2. It is seen that the self-sustaining premixed flame section features a strong post-reaction zone structure as shown in dark blue colors, while the flame hole's post-reaction zone is mostly suppressed (thus the flame is not self-sustaining) as indicated by the light blue colors. The flame hole is further evident on the species explosion index (EI) plot. The EI value of a species indicates the normalized contribution of a species to the local explosive mode. It is seen that the controlling species (those with large EI values) are dramatically different for strongly burning flames vs. the flame hole, showing that the controlling chemistry will change in a flame once local extinction occurs.

The CEMA-based criteria are therefore shown to be effective and can be extended as computational diagnostics to systematically detect and track local ignition, extinction and reaction fronts in complex turbulent flame fields, providing a robust local flame marker for switching between different turbulent combustion models that are suitable for different local flame features.

2. Effects of surrogate components on jet fuel ignition and extinction and a bifurcation analysis

Jet fuels involve a large number of components with different molecular structures, e.g. alkanes, alkenes and aromatics, primarily ranging from C7 to C16. It is computationally expensive to solve such a large number of fuel species and the myriad intermediate species and reaction pathways associated with these fuel components in turbulent flame simulations. As such, surrogate mixtures with one or a few surrogate components are frequently employed to develop chemical kinetic models to capture the major properties of the real fuels, e.g. the distillation curves, thermodynamic properties, ignition and extinction behaviors, and flame speeds. In the present project, the viability of using a single-component surrogate to capture high-temperature

jet fuel combustion features (ignition and extinction) was computationally explored, with the results explained using a rigorous bifurcation analysis.

Three types of hydrocarbons, including normal-alkanes, cyclo-alkanes, and aromatics are considered as primary jet fuel surrogate components in the present study. It was found that normal-alkanes with different chain lengths (C8~C12) and branched cyclo-alkane (represented by n-butyl cyclohexane) show similar ignition and extinction behaviors in high-temperature combustion (e.g. above 1000K). As such pure n-dodecane can be an adequate representative component for the normal- and cyclo-alkanes components in jet fuels in terms of capturing high-temperature ignition and extinction behaviors.

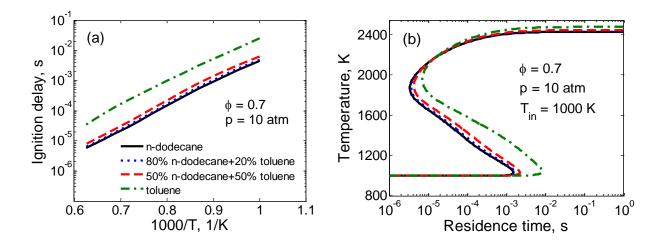


Figure 3: (a) Ignition delay time as a function of initial temperature in constant-pressure autoignition, and (b) the *S*-curves of perfectly stirred reactors (PSRs), for n-dodecane, toluene, and binary mixtures of n-dodecane and toluene with 0, 20%, and 50% toluene in mole, respectively.

It was further shown in Fig. 3 that, while pure aromatics (e.g. toluene) features significantly ignition and extinction properties from n-dodecane, blending a small to moderate amount of toluene (say up to 50% in mole) in n-dodecane only induces minor changes in the

ignition and extinction states. This result indicates that pure n-dodecane can be a sufficiently accurate jet fuel surrogate for high-T ignition and extinction, such that a simple chemical kinetic mechanism for pure n-dodecane can be adequate to accurately predict high-T ignition and extinction of jet fuels.

To explain the underlying reasons for this observation, a bifurcation analysis is employed to identify the controlling species and reactions for jet fuel ignition and extinction. The bifurcation analysis is focused on (quasi-) steady flames that feature the combustion S-curves. The upper turning point of the S-curve is corresponding to the extinction state and the lower turning point to the ignition state. The extinction and ignition states are important for flame stabilization and are mathematically described as bifurcation points associated with zero-crossing eigenvalues of the Jacobian matrix. The controlling reactions of the ignition and extinction can therefore be identified by quantifying the contribution of each species and reaction to the zero-crossing of the eigenvalue, and such normalized contribution from a reaction to the bifurcation is defined as the bifurcation index (BI), which is used in the present study to subsequently identify the controlling reactions for ignition and extinction.

The reactions and the mixing process with large BI values are listed in Figs. 4a and b for the extinction and ignition states, respectively. Fig. 4a shows that the extinction states of the different binary mixtures with different amounts of toluene addition are controlled by the mixing process and a set of reactions involving small molecules that are relevant to CO formation and the hydrogen chemistry, while the reactions for fuel cracking for either n-dodecane or toluene do not play a significant role at the extinction state. At the ignition state, it is shown in Fig. 4b that the controlling reactions for the different mixtures primarily involve ethylene, vinyl radical, alkyl radical and other small species that are important intermediate products of beta-scission. The results in Fig. 4 indicate that, since fuel cracking through beta-scission becomes exceedingly fast

at high temperatures, they are not rate-limiting at either the extinction or the ignition states. As such, it is possible to capture high-T jet fuel ignition an extinction behaviors using lumped fuel cracking reactions, such that the jet fuel chemistry can be significantly simplified and expedited for time integration at high-T flame simulations.

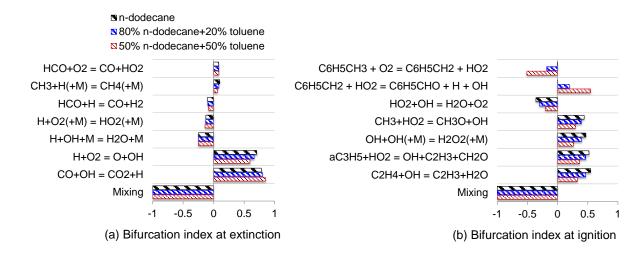


Figure 4: Reactions ranked in bifurcation index (BI) for the (a) extinction and (b) ignition states on the *S*-curves of perfectly stirred reactors (PSRs) in Fig. 3b for the binary mixtures of n-dodecane and toluene.

3. Reduced mechanisms for n-butane and n-dodecane with lumped fuel cracking reactions

Detailed chemistry is an integral component of turbulent flame simulations. As such an accurate and efficient chemistry description is critical for CFD predictions. To develop highly efficient yet still accurate reduced mechanisms for jet fuel combustion, the above observation for the fuel cracking is exploited and the fuel cracking reactions are lumped (in collaboration with Hai Wang) to significantly reduce the amount of intermediate species generated during fuel cracking. Two fuels, namely n-butane and n-dodecane, are selected for the reduction: n-butane was selected as it is the smallest alkane that features clear fuel cracking pathways, while n-

dodecane was selected as it is an important jet fuel surrogate for high-T flame conditions as discussed above.

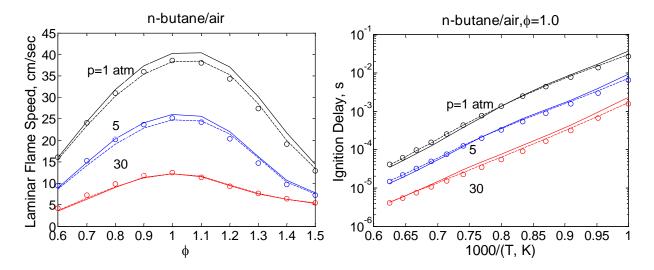


Figure 5: Validation of the lumped and reduced mechanisms for n-butane/air: a) laminar flame speed, and b) ignition delay time at different pressures and equivalence ratios. Solid lines: detailed USC-Mech II; dashed lines: lumped fuel cracking reactions; symbols: 28-species reduced.

The detailed USC-Mech II mechanism with 111 species is used as the starting mechanism for n-butane. The fuel cracking reactions were first lumped (by Hai Wang and student), resulting in a 58-species mechanism. Systematic mechanism reduction methods based on directed relation graph (DRG), sensitivity analysis and quasi steady state approximations (QSSA) were further employed to reduce the mechanism to 28 species. The detailed, lumped and reduced mechanisms are compared in Fig. 5 for flame speed and ignition delays, and close agreement was observed for the displayed and other flame conditions.

For n-dodecane, a JetSurF mechanism (from Hai Wang's group) with 123 species and lumped fuel cracking reactions was employed as the starting mechanism. The reduction covered auto-ignition and perfectly stirred reactors for equivalence ratio range of 0.5~1.5, initial temperature higher than 1000 K, and at atmospheric pressure. The reduced mechanism consists

of only 24 species, with the high accuracy of the reduced mechanism shown in Fig. 6. The effectiveness to use lumped fuel cracking steps to simplify high-T jet fuel chemistry is therefore evident.

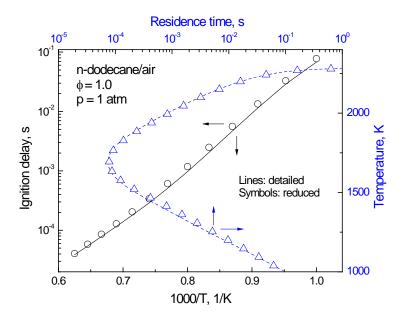


Figure 6: Ignition delay as a function of initial temperature in constant-pressure auto-ignition (bottom-left) and temperature as a function of residence time in PSR with inlet temperature of 300 K (top-right), for stoichiometric n-dodecane/air at atmospheric pressure, calculated with the detailed and reduced mechanisms, respectively.

4. 2-D DNS of premixed turbulent n-butane flames

To further study the effects of fast turbulent mixing on fuel cracking reactions, 2-D DNS for premixed n-butane/air flames (equivalence ratio = 0.6) were performed in the thin reaction zones regime and the broken reaction zones regime, respectively. The flames are initialized with the 1-D premixed flame profile and isotropic turbulence, and the flames propagate into fresh mixtures at 500K at a pressure of 5 atm, with the flame fronts disturbed by the turbulence fluctuations. The computational domain is 10mm by 15mm with 5 uniform grid points.

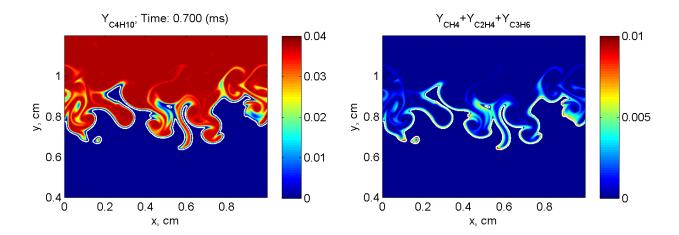


Figure 7: DNS of a 2-D premixed n-butane/air flame in the broken reaction zones regime: a) the fuel concentration and b) the concentrations of selected fuel cracking products at t = 0.7ms. The white isolines are the premixed reaction fronts (eigenvalue zero-crossing) identified by CEMA.

The flame structure at t = 0.7ms for the case in the broken-reaction zones regime is shown in Fig. 7. The DNS results show that despite the strong turbulent mixing, fuel molecules have never been observed to penetrate into the reaction zone of the flames indicated by the white isolines in Fig. 7, and the fast fuel cracking assumption is valid for flames even with strong turbulent mixing. Further statistical analysis of the DNS data shows that the fuel cracking reactions are mostly complete at temperature between 1500 K and 1600 K, as such the lumped fuel cracking reactions do not have significant effects on the chemistry in the reaction zones in the strongly turbulent premixed flames.

5. Fuel cracking in near-extinction flames

To further study the validity of fuel cracking lumping under extreme combustion conditions, such as in near-extinction flames, the flame responses to the flow strain was tested in

1-D counterflow non-premixed and premixed flames using the detailed JetSurF 1.0, lumped-detailed model (JetSurF 1.0-l) and the 24-species reduced n-dodecane model.

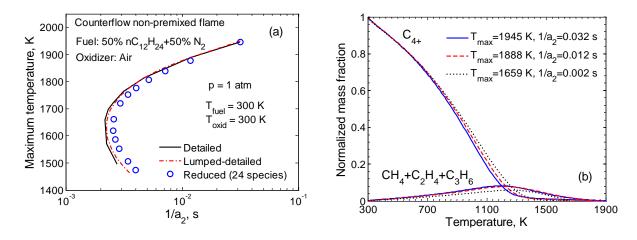


Figure 8: (a) Comparison of the maximum temperature $T_{\rm max}$ in counterflow non-premixed flames as a function of the strain rate, calculated with the detailed, lumped-detailed and 24-species reduced models; (b) Normalized total mass fraction of C_{4+} species, and that of the primary fuel cracking products, including CH_4 , C_2H_4 and C_3H_6 , at three different strain rates as predicted by the detailed model. The flames are at atmospheric pressure and an inlet temperature of 300 K with the fuel jet comprised of 50% (mol) n-dodecane in N_2 and air at 300 K as the oxidizer jet.

Figure 8a shows the maximum temperature, computed for the non-premixed counterflow flames as a function of the strain rate a_2 . It is seen that, the lumped model agrees well with the detailed model over the entire curves, including the turning point, which corresponds to the extinction state of the flames. In worst case, the 24-species reduced model gives an error about 20% in the extinction strain rate. Figure 8b shows the normalized total mass fraction of species with four or more carbon atoms, C_{4+} and the primary fuel cracking products, CH_4 , C_2H_4 , and C_3H_6 . The three profiles shown in Figure 8b were calculated with rather different strain rates, spanning from strongly burning to extinction states. The fuel cracking behaviors are quite similar

for all these strain rates. Specially, the C_{4+} species primarily vanish by about 1500 K, indicating that the fuel cracking process is completed in the preheat zone before the main flame zone. Accordingly, the fuel cracking products are oxidized in the main flame zone.

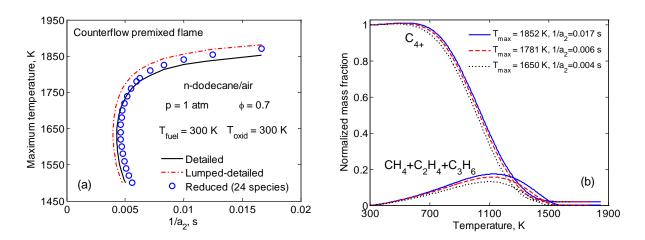


Figure 9: (a) Comparison of maximum temperature $T_{\rm max}$ in counterflow premixed flames as a function of the strain rate, calculated with the detailed, lumped-detailed and 24-species reduced models; (b) Normalized total mass fraction of C_{4+} species, and that of the primary fuel cracking products, including CH_4 , C_2H_4 and C_3H_6 , at three different strain rates as predicted by the detailed model. The flames are at atmospheric pressure and an inlet temperature of 300 K with the twin jets composed of an n-dodecane/air mixture at equivalence ratio 0.7.

Figure 9 shows extinction of premixed counterflow flames predicted using both the lumped-detailed and the 24-species reduced models. The results are close to that of the detailed model, including the near extinction states. Comparison of the premixed and non-premixed counterflow results show similar features. In all cases, fuel cracking is completed before 1500 K. Overall, the lumping approach is shown to be valid for premixed and non-premixed flames at near-extinction conditions.

6. A dynamic adaptive hybrid method for stiff chemistry integration (AHI)

Detailed chemical kinetic models are expensive to be accommodated in CFD simulations due to not only the large sizes but also severe chemical stiffness, which renders the low cost explicit time integration solvers infeasible unless extremely small integration time steps are assumed. As such, implicit solvers are typically employed in LES and RANS, and DNS of incompressible flows. However, fully implicit integration solvers are computationally prohibitive for multi-dimensional flow simulations, and operator splitting schemes are widely used to separate the integration of chemical and flow processes into sequential sub-steps. It was found that, for systems with significant radical sources from transport, splitting chemistry from transport may induce O(1) errors. Similar splitting errors were also identified for extinction problems. To solve the problem, a dynamic adaptive hybrid integration (AHI) method for stiff chemistry integration was developed. In AHI, chemistry and transport are integrated together to avoid the splitting errors. Only fast species and fast reactions are solved implicitly while the other variables and source terms are treated explicitly to reduce the computational cost. Furthermore, an improved second order AHI scheme (AHI2) was developed to achieve higher accuracy. Figure 10 shows the comparison of solutions of a toy problem using AHI and the Strang splitting scheme, respectively. The toy problem involves rate controlling reactions with O(1) timescales and a radical with 10^{-6} timescale. Figure 11 compares errors in the Strang splitting, AHI and AHI2, respectively, for the toy problem. It is seen that the Strang splitting scheme gives O(1)errors unless the integration time step is close to or shorter than that required for explicit solvers, while AHI accurately predicts the species concentrations with significantly higher accuracy. AHI2 achieved even higher accuracy over a wide range of integration time steps.

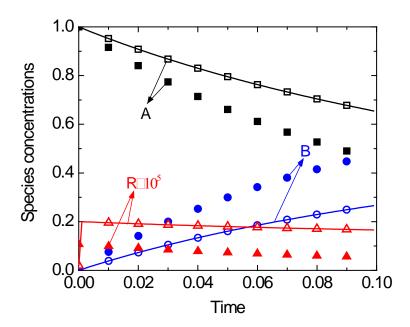


Figure 10: Profiles of species concentrations in a toy problem, calculated with the first-order AHI method (open symbols) and the Strang splitting scheme, respectively, in comparison with the exact solution (lines). Time steps for Strang splitting and AHI are both 10⁻⁵.

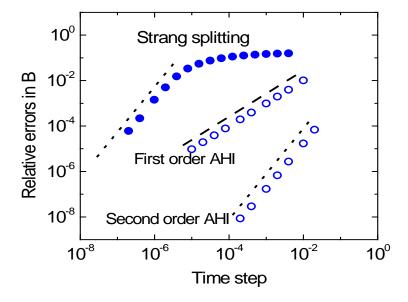


Figure 11: Error control behavior for Strang splitting, first-order AHI and second-order AHI in the toy problem. The dotted line is a trend line with a slope of 2, indicating second-order accuracy. The dashed line is a trend line with a slope of 1, indicating first-order accuracy.

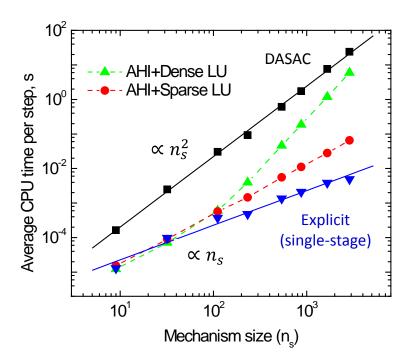


Figure 12: Average CPU time per step for fully implicit DASAC, one-stage explicit solver, AHI with dense LU decomposition, and AHI with sparse LU decomposition, respectively.

In term of computational efficiency, Fig. 12 further compares the fully implicit DASAC solver, one-stage fully explicit solver, AHI with dense LU decomposition, and AHI with sparse LU factorization. It is seen that AHI with dense LU can achieve O(10)-O(100) speedup factors for mechanisms of different sizes, while AHI with sparse LU factorization can achieve comparable cost linearly proportional to the mechanism size, being comparable to the highly efficient single-stage explicit solver.

MAJOR PUBLICATIONS

- 1. Shan R., Lu T.F., "A Bifurcation Analysis for Limit Flame Phenomena of DME/air in Perfectly Stirred Reactors," Combustion and Flame, Vol. 161, No. 7, pp. 1716–1723, 2014.
- 2. Gao Y., Liu Y., Ren Z., Lu T.F., "A dynamic adaptive method for hybrid integration of stiff chemistry", Combustion and Flame, Vol. 161, No. 2, pp. 287–295, 2015.
- 3. Vie A., Franzelli B. Gao Y., Lu T.F., Wang H., Ihme M., "Analysis of segregation and bifurcation in turbulent spray flames: A 3D counterflow configuration," Proceedings of the Combustion Institute, Vol. 35, No. 2, pp. 1675–1683, 2015.
- 4. Gao Y., Shan R., Lyra S., Li C., Wang H., Chen J.H., Lu T.F., "On lumped-reduced reaction model for combustion of liquid fuels", Combustion and Flame, submitted.
- 5. Ren Z., Gao Y., Lu Z., Lu T.F., Hou L., "A Kinetics-Based Method for Constraint Selection in Rate-Controlled Constrained Equilibrium," Combustion and Flame, submitted.

PUBLIC PRESENTATIONS

- Gao Y., Xu C., Ren Z., Lu T.F., "A second-order dynamic adaptive hybrid scheme for stiff chemistry integration," Paper # 114TF-0084, 9th U.S. National Combustion Meeting, Cincinnati, Ohio, May 17-20, 2015.
- Gao Y., Shan R., Lyra S., Li C., Wang H., Chen J.H., Lu T.F., "Development of reduced mechanisms with lumped reactions for fuel cracking for high-temperature combustion of practical fuels," Paper # 114RK-0058, 9th U.S. National Combustion Meeting, Cincinnati, Ohio, May 17-20, 2015.

- 3. Xu C., Gao Y., Ren Z., Lu T.F., "A sparse stiff chemistry solver based on dynamic adaptive hybrid integration for efficient combustion simulations," Paper # 114RK-0092, 9th U.S. National Combustion Meeting, Cincinnati, Ohio, May 17-20, 2015.
- 4. Shan R., Lu T.F., "A Kinetic Model for Limit Phenomena Prediction Based on Bifurcation Analysis," 4th International Workshop on Model Reduction in Reacting Flows, Marriott Marquis Hotel, San Francisco, California, June 19–21, 2013.
- Shan R., Lu T.F., "Effects of Surrogate Jet-Fuel Composition on Ignition and Extinction in High Temperature Applications," Paper # 070LT-0077, 8th U. S. National Combustion Meeting, Park City, Utah, May 19-22, 2013.

PERSONNEL

- 1. Tianfeng Lu (Principal Investigator)
- 2. Zhuyin Ren (Co-PI, Visiting Assistant Professor, University of Connecticut)
- 3. Jacqueline H. Chen (Co-PI, Distinguished Member of Technical Staff, Sandia National Laboratories)
- 4. Hai Wang (Collaborator, Stanford University)
- 5. David Lignell (Collaborator, Assistant Professor, Brigham Young University)
- 6. Sgouria Lyra (Collaborator, Postdoc, Sandia CRF)
- 7. Xianming Wang (Postdoc at UConn)
- 8. Ruiqin Shan (Ph.D. student graduated from UConn)
- 9. Mike Kuron (4rd year Ph.D. student at UConn)
- 9. Yunchao Wu (3nd year Ph.D. student at UConn)
- 10. Cong Li (M.S. student graduated from UConn)
- 11. Yang Gao (2nd year Ph.D. student at UConn)

TECHNOLOGY TRANSITIONS

1. <u>Performer</u>: Tianfeng Lu, University of Connecticut; 860-486-3942

Customer: Taitech, Inc., AFRL/RQHF contractor, (Dr. Jiwen Liu, 937-255-3560)

Results: Use of compressively reduced chemical kinetic mechanisms for high speed

turbulent flame simulations.

Applications: flame simulations with systematically reduced chemistry.

2. Performer: Zhuyin Ren and Tianfeng Lu, University of Connecticut, 860-486-3942

Customer: Fluent, Inc., (Graham Goldin, 800-445-4454)

Results: Use of directed relation graph based on dynamic adaptive chemistry of

realistic fuel chemistry in flame simulations with Fluent.

Applications: Building highly efficient dynamic adaptive chemistry in the commercial

Fluent code for general flame simulations.

3. <u>Performer:</u> Tianfeng Lu and Zhuyin Ren, University of Connecticut, 860-486-3942

Customer: CD-Adapco, (Dr. Rajesh Rawat, 631-549-2300, ext. 25143)

Results: Use of directed relation graph and analytic Jacobian techniques for highly

efficient flame simulations with realistic chemistry.

Applications: Building DRG based dynamic adaptive chemistry and analytic Jacobian

techniques in the commercial Star-CCM+ code for general flame

simulations.

PRINCIPAL INVESTIGATOR ANNUAL DATA COLLECTION (PIADC) SURVEY

PI DATA

Name Tianfeng Lu

<u>Institution</u> University of Connecticut

Grant No. FA9550-13-1-0057

NUMBER OF CONTRACT/GRANT CO-INVESTOGATORS

Faculty: 2

Post Doctorates: 1

Graduate Students: 5

Other: 3 (Collaborators at no cost to grant)

PUBLICATIONS RELATED TO AFOREMENTIONED CONTRACT/GRANT

Name of Journal: Combustion and Flame

<u>Title</u>: A Bifurcation Analysis for Limit Flame Phenomena of DME/air in Perfectly Stirred Reactors

Authors: Ruiqin Shan, and Tianfeng Lu

DOI: http://dx.doi.org/10.1016/j.combustflame.2013.12.025 Year Published: 2014

Name of Journal: Combustion and Flame

<u>Title</u>: A dynamic adaptive method for hybrid integration of stiff chemistry

Authors: Yang Gao, Yufeng Liu, Zhuyin Ren, and Tianfeng Lu

DOI: http://dx.doi.org/10.1016/j.combustflame.2014.07.023 Year Published: 2015

Name of Journal: Proceedings of the Combustion Institute

<u>Title:</u> Analysis of segregation and bifurcation in turbulent spray flames: A 3D counterflow configuration

<u>Authors</u>: Aymeric Vié, Benedetta Franzelli, Yang Gao, Tianfeng Lu, Hai Wang, and Matthias Ihme

<u>DOI</u>: http://dx.doi.org/10.1016/j.proci.2014.06.083 <u>Year Published</u>: 2015

HONORS/AWARDS RECEIVED DURING CONTRACT/GRANT LIFETIME

Honor/Award: Associated Fellow of AIAA

Year Received: 2014

Honor/Award Recipient: Tianfeng Lu

Awarding Organization: AIAA